

=> fil reg

FILE 'REGISTRY' ENTERED AT 12:01:53 ON 15 APR 2004  
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STRUCTURE FILE UPDATES: 14 APR 2004 HIGHEST RN 675571-70-7  
 DICTIONARY FILE UPDATES: 14 APR 2004 HIGHEST RN 675571-70-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

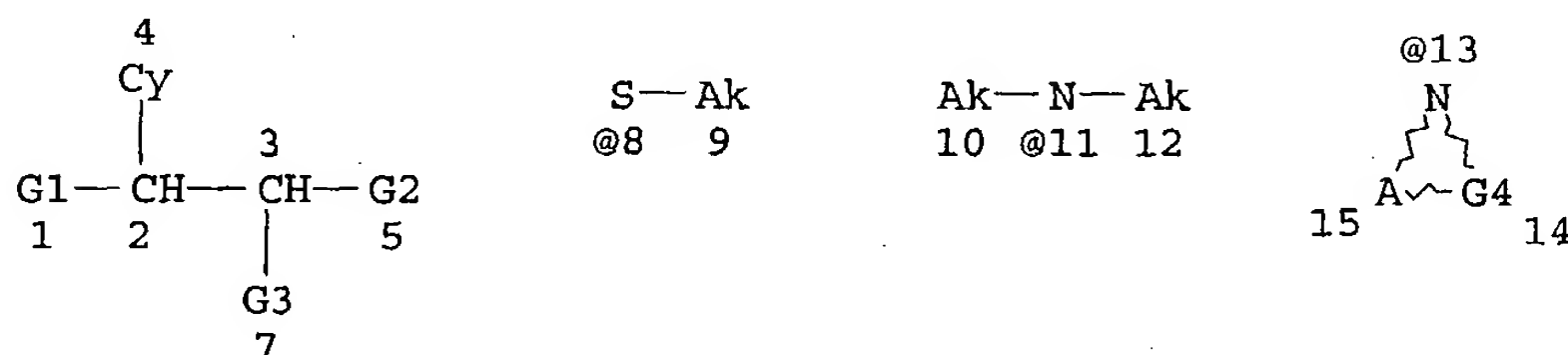
Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
 information enter HELP PROP at an arrow prompt in the file or refer  
 to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que 127

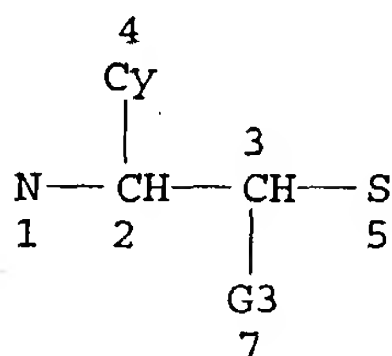
L12 STR



VAR G1=11/13  
 VAR G2=S/8  
 VAR G3=AK/CB  
 REP G4=(1-6) A  
 NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RSPEC 13  
 NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE  
 L21 SCR 1164  
 L23 STR

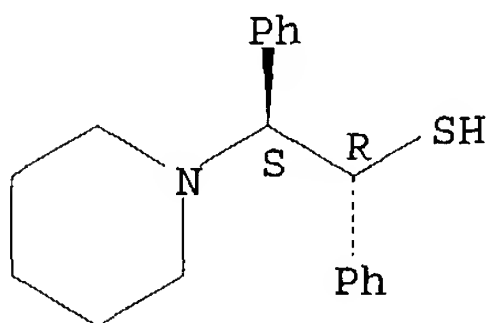


VAR G3=AK/CB  
 NODE ATTRIBUTES:  
 NSPEC IS RC AT 1  
 DEFAULT MLEVEL IS ATOM

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ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1997:39785 CAPLUS  
DOCUMENT NUMBER: 126:131036  
TITLE: Chiral  $\beta$ -amino thiol catalysts for the  
enantioselective addition of diethylzinc to aldehydes  
AUTHOR(S): Kang, Jahyo; Kim, Jeong Whan; Lee, Jun Won; Kim, Dong  
Soo; Kim, Joo In  
CORPORATE SOURCE: Dep. Chem., Sogang Univ., Seoul, 121-742, S. Korea  
SOURCE: Bulletin of the Korean Chemical Society (1996),  
17(12), 1135-1142  
CODEN: BKCSDE; ISSN: 0253-2964  
PUBLISHER: Korean Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Reaction of diethylzinc with  $\alpha$ -branched aldehydes in the presence of  
a catalytic amount (5 mol %) of various  $\beta$ -amino thiols in toluene or  
ether provided the corresponding secondary alcs. in outstanding ee.  
Detailed preparative procedure for the  $\beta$ -amino thiols are presented.  
IT 160011-80-3P  
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent); USES (Uses)  
(enantioselective addition of diethylzinc to aldehydes using chiral  
 $\beta$ -amino thiol catalysts)  
RN 160011-80-3 CAPLUS  
CN 1-Piperidineethanethiol,  $\alpha,\beta$ -diphenyl-, ( $\alpha R,\beta S$ )-  
(9CI) (CA INDEX NAME)

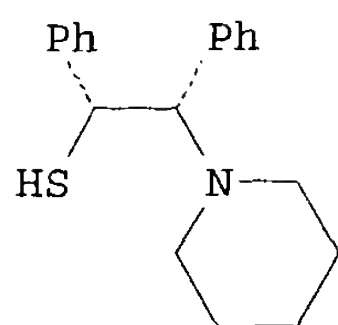
Absolute stereochemistry. Rotation (-).



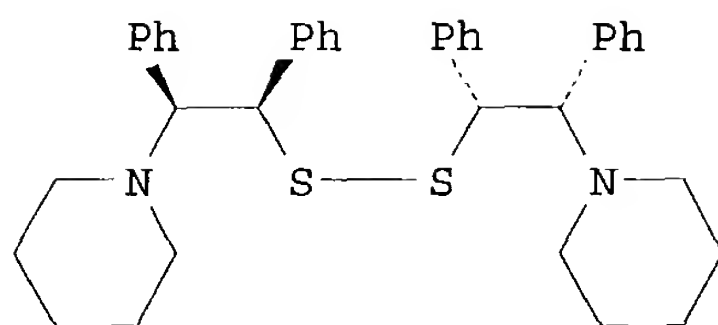
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1995:194984 CAPLUS  
DOCUMENT NUMBER: 122:55341  
TITLE: Enantioselective addition of diethylzinc to aldehydes  
catalyzed by a drug-unrelated chiral amino thiol and  
the corresponding disulfide  
AUTHOR(S): Kang, Jahyo; Kim, Dong Soo; Kim, Joo In  
CORPORATE SOURCE: Department Chemistry, Sogang University, Seoul,  
121-742, S. Korea  
SOURCE: Synlett (1994), (10), 842-4  
CODEN: SYNLES; ISSN: 0936-5214  
PUBLISHER: Thieme  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 122:55341  
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I



II

AB Reaction of diethylzinc with aldehydes in the presence of a catalytic amount of a  $\beta$ -amino thiol I (5 mol %) and the disulfide II (2.5 mol %) in toluene at 0° provided the corresponding secondary alcs. in excellent ee's.

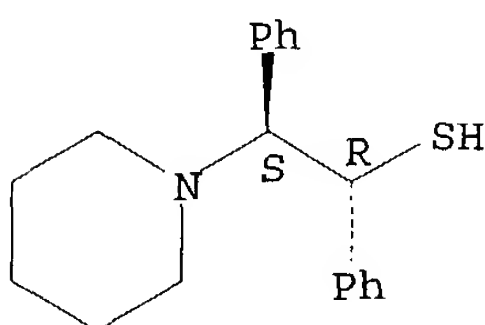
IT 160011-80-3P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(enantioselective addition of diethylzinc with aldehydes catalyzed by chiral amino thiol and disulfide)

RN 160011-80-3 CAPLUS

CN 1-Piperidineethanethiol,  $\alpha,\beta$ -diphenyl-, ( $\alpha$ R, $\beta$ S)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



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L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1990:531411 CAPLUS  
DOCUMENT NUMBER: 113:131411  
TITLE: Concerning mass spectra of  $\beta$ -heterosubstituted  
thioethers  
AUTHOR(S): Carreno, M. Carmen; Carretero, Juan C.; Garcia Ruano,  
Jose L.; Martinez, M. Carmen  
CORPORATE SOURCE: Dep. Quim., Univ. Auton. Madrid, Madrid, 28049, Spain  
SOURCE: Organic Mass Spectrometry (1990), 25(6), 339-42  
CODEN: ORMSBG; ISSN: 0030-493X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The mass spectra of 32 erythro- and threo-RCHXCHRSMe (R = Me, Ph; X = F,  
Cl, Br, iodo, OH, OMe, OAc, NH<sub>2</sub>, NMe<sub>2</sub>) were interpreted in detail. Linear  
free-energy relationships were determined between the ratio of the relative  
abundances of the RCHX<sup>+</sup> and RCHSMe<sup>+</sup> peaks and the inductive and resonance  
 $\sigma$  consts. of X.  
IT 97241-47-9  
RL: PRP (Properties)  
(mass spectrum of)  
RN 97241-47-9 CAPLUS  
CN Benzeneethanamine, N,N-dimethyl- $\beta$ -(methylthio)- $\alpha$ -phenyl-,  
(R\*,R\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

